1. Record Nr. UNINA9910971990603321

Autore	Nakamura Hiroki
Titolo	Quantum mechanical tunneling in chemical physics / / Hiroki Nakamura, Gennady Mil'nikov
Pubbl/distr/stampa	Boca Raton, : CRC Press, Taylor & Francis Group, 2013 Boca Raton : , : CRC Press, Taylor & Francis Group, , 2013
ISBN	1-04-019274-2 0-429-08645-8 1-4665-0731-4
Edizione	[1st ed.]
Descrizione fisica	1 online resource (225 p.)
Classificazione	SCI013050SCI078000
Disciplina	537.6/226
Soggetti	Tunneling (Physics)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Front Cover; Quantum Mechanical Tunneling in Chemical Physics; Copyright; Table of Contents; Preface; 1. Introduction; 2. One-Dimensional Theory; 3. Two-Dimensional Theory; 4. Multidimensional Effects: Peculiar Phenomena; 5. Nonadiabatic Tunneling; 6. Multidimensional Theory of Tunneling Splitting; 7. Numerical Applications to Polyatomic Molecules; 8. Decay of Metastable States; 9. Tunneling in Chemical Reactions; 10. Concluding Remarks and Future Perspectives; Appendix A: Proofs of Equation (2.95) and Equation (2.110); Appendix B: Derivation of Equation (6.80) Appendix C: Herring Formula in Curved SpaceAppendix D: Derivation of Equation (6.97); Appendix E: Computer Code to Calculate Instanton Trajectory; Appendix F: Derivation of Some Equations in Section 6.4.2; Bibliography; Back Cover
Sommario/riassunto	This text explores methodologies that can be usefully applied to various realistic problems in molecular spectroscopy and chemical dynamics. It covers the direct evaluation of reaction rate constants for both electronically adiabatic chemical reactions on a single adiabatic potential energy surface and non-adiabatic chemical reactions in which two or more adiabatic potential energy surfaces are involved. It also discusses the non-adiabatic tunneling phenomenon that represents

one class of non-adiabatic transitions on which the authors have made an extensive research so far--